

Quantum States and Hardy's Formulation of the Uncertainty Principle : a Symplectic Approach

Maurice de Gosson Franz Luef
 Faculty of Mathematics, University of Vienna
 Nordbergstrasse 15
 A-1090 Vienna
 maurice.de.gosson@univie.ac.at
 franz.luef@univie.ac.at

February 1, 2008

Abstract

We express the condition for a phase space Gaussian to be the Wigner distribution of a mixed quantum state in terms of the symplectic capacity of the associated Wigner ellipsoid. Our results are motivated by Hardy's formulation of the uncertainty principle for a function and its Fourier transform. As a consequence we are able to state a more general form of Hardy's theorem.

MSC 2000 Classification: 81S10, 81S30, 37J05

1 Introduction

In the early days of quantum mechanics Heisenberg made the fundamental observation that the position of an electron and its momentum cannot be measured simultaneously with arbitrary precision. Since then many attempts have been undertaken to turn Heisenberg's uncertainty principle into rigorous mathematical theorems. The most well-known interpretation is due to Born which expresses Heisenberg's principle in terms of non-commutativity of a pair of operators. More precisely, defining the *position operator* X and *momentum operator* P by $X\psi = x \cdot \psi$ and $P\psi = -i\hbar\partial_x\psi$ (ψ in some adequate dense subspace of $L^2(\mathbb{R})$) Heisenberg's uncertainty principle is reflected by the non-commutativity of the position and momentum

¹The authors were supported under the EU-project MEXT-CT-2004-51715.

operator,

$$XP - PX = i\hbar I.$$

In his trailblazing work on the mathematical foundations of quantum mechanics Weyl, inspired by Born's probabilistic interpretation of physical states in quantum mechanics, showed that the non-commutativity of position and momentum operator is actually a statement about the variances of X and P :

$$\left(\int_{-\infty}^{\infty} x^2 |\psi(x)|^2 dx \right)^{1/2} \left(\int_{-\infty}^{\infty} \hbar^2 |\partial_x \psi(x)|^2 dx \right)^{1/2} \geq \frac{1}{2} \|\psi\|^2. \quad (1)$$

Recently one of us [5, 7] has pointed out a formulation of the uncertainty principle in terms of covariance matrices which has several attractive features and consequences. We will return to this fact later since it is one of our tools to extend Hardy's theorem to the higher-dimensional setting. We continue with our short historical overview. Wiener observed that Weyl's formulation of Heisenberg's uncertainty principle means that a quantum state ψ and its Fourier transform cannot both be well-localized in phase space. In [10] Hardy obtained the following theorem which turned Wiener's observation into a rigorous mathematical statement. Defining the Fourier transform of $\psi \in L^2(\mathbb{R})$ by

$$\mathcal{F}\psi(p) = \left(\frac{1}{2\pi\hbar} \right)^{1/2} \int_{-\infty}^{\infty} e^{-\frac{i}{\hbar} px} \psi(x) dx$$

and noting that $\psi_0(x) = e^{-x^2}$ is a minimizer of (1), Hardy suggested to measure the localization of ψ and $\mathcal{F}\psi$ with respect to a Gaussian:

Theorem 1 (Hardy, [10]) *Let ψ be in $L^2(\mathbb{R})$. If there exist constants $C_X, C_P > 0$ and $a, b > 0$ such that*

$$|\psi(x)| \leq C_X e^{-\frac{a}{2\hbar} x^2} \quad \text{and} \quad |\mathcal{F}\psi(p)| \leq C_P e^{-\frac{b}{2\hbar} p^2} \quad (2)$$

then: (i) If $ab = 1$, there exists $C \in \mathbb{C}$ such that $\psi(x) = Ce^{-\frac{a}{2\hbar} x^2}$. (ii) If $ab > 1$, then ψ vanishes identically. (iii) If $ab < 1$ then the set of functions satisfying (2) is non-empty (it contains all conveniently rescaled Hermite functions).

Hardy's theorem has been generalized and extended to various settings in mathematics and physics (with, for instance, the Gaussian replaced by some other exponential functions, and the phase space by some Lie group: see [19]). Despite the vast literature on Hardy's formulation of Heisenberg's

uncertainty principle we are not aware of any approach which provides an explanation of the parameters a and b . In the present paper we discuss Hardy's theorem in terms of symplectic geometry. Therefore we are able to invoke notions of symplectic topology such as the symplectic capacity of a phase space ellipsoids.

We will do the following in this Letter:

- We will formulate Hardy's theorem in terms of the notion of symplectic capacity $c(\mathcal{B}_M)$ of a phase-space ellipsoid $\mathcal{B}_M : Mz \cdot z \leq 1$; that capacity is expressed in terms of an invariant associated to the Williamson diagonal form of M ;
- We will apply this result to a characterization of the (cross)-Wigner distribution of Gaussian states which are localized on an ellipse in phase space, and obtain an useful estimate. As a by-product we will prove that a Wigner distribution can never have compact support.

Notation. The symplectic product of two vectors $z = (x, p)$, $z' = (x', p')$ in \mathbb{R}^{2n} is $\sigma(z, z') = p \cdot x' - p' \cdot x$ where the dot \cdot is the usual (Euclidean) scalar product on \mathbb{R}^n . In matrix notation:

$$\sigma(z, z') = (z')^T J z \quad , \quad J = \begin{pmatrix} 0_{n \times n} & I_{n \times n} \\ -I_{n \times n} & 0_{n \times n} \end{pmatrix}.$$

The corresponding symplectic group is denoted by $\text{Sp}(n, \mathbb{R})$: the relation $S \in \text{Sp}(n, \mathbb{R})$ means that S is a real $2n \times 2n$ matrix such that $\sigma(Sz, Sz') = \sigma(z, z')$; equivalently $S^T J S = S J S^T = J$.

For $(\psi, \phi) \in L^2(\mathbb{R}^n) \times L^2(\mathbb{R}^n)$ the Wigner–Moyal transform (or: distribution) $W(\psi, \phi)$ is defined by

$$W(\psi, \phi)(x, p) = \left(\frac{1}{2\pi\hbar}\right)^n \int_{\mathbb{R}^n} e^{-\frac{i}{\hbar} p \cdot y} \psi\left(x + \frac{1}{2}y\right) \overline{\phi\left(x - \frac{1}{2}y\right)} dy; \quad (3)$$

the function $W\psi = W(\psi, \psi)$ is the Wigner transform (or: distribution) of ψ .

For $z_0 = (x_0, p_0)$ the Heisenberg–Weyl operator $\hat{T}(z_0)$ is defined by

$$\hat{T}(z_0)\psi(x) = e^{\frac{i}{\hbar}(p_0 \cdot x - \frac{1}{2}p_0 \cdot x_0)} \psi(x - x_0).$$

2 Canonical formulation of the uncertainty principle

In what follows A and B are two (essentially) self-adjoint operators on $L^2(\mathbb{R}^n)$ with domains D_A and D_B . For $\psi \in D_A$, $\|\psi\|_{L^2} = 1$ we set $\langle A \rangle_\psi = (A\psi, \psi)_{L^2}$.

Assume that the (co-)variances

$$\begin{aligned} (\Delta A)_\psi^2 &= \langle A^2 \rangle_\psi - \langle A \rangle_\psi^2, \quad (\Delta B)_\psi^2 = \langle B^2 \rangle_\psi - \langle B \rangle_\psi^2 \\ \Delta(A, B)_\psi &= \frac{1}{2} \langle AB + BA \rangle_\psi - \langle A \rangle_\psi \langle B \rangle_\psi \end{aligned}$$

exist. Then (see for instance Messiah [15])

$$(\Delta A)_\psi^2 (\Delta B)_\psi^2 \geq \Delta(A, B)_\psi^2 - \frac{1}{4} \langle [A, B] \rangle_\psi^2. \quad (4)$$

The proof of this inequality is based on the trivial identity

$$AB = \frac{1}{2}(AB + BA) + \frac{1}{2}(AB - BA);$$

notice that since $(AB + BA)^* = AB + BA$ and $[A, B]^* = -[A, B]$ we have $\Delta(A, B)_\psi^2 \geq 0$ and $\langle [A, B] \rangle_\psi^2 \leq 0$ so that (4) implies that

$$(\Delta A)_\psi (\Delta B)_\psi \geq -\frac{1}{4} \langle [A, B] \rangle_\psi^2 \geq 0.$$

It is this weak form of the uncertainty principle, obtained by neglecting correlations, that is almost exclusively discussed in the mathematical literature. This is indeed a pity, because one then loses one of the most interesting and useful features of the uncertainty principle, namely its canonical invariance.

Specializing to the case where A and B are the operators X_j and P_j defined, for $\psi \in \mathcal{S}(\mathbb{R}^n)$, by $X_j\psi = x_j\psi$ and $P_j\psi = -i\hbar\partial_{x_j}\psi$. Schrödinger's formulation (4) of Heisenberg's uncertainty principle becomes in this case

$$(\Delta X_j)_\psi^2 (\Delta P_j)_\psi^2 \geq \Delta(X_j, P_j)_\psi^2 + \frac{1}{4}\hbar^2, \quad 1 \leq j \leq n \quad (5)$$

$$(\Delta X_j)_\psi^2 (\Delta P_k)_\psi^2 \geq \Delta(X_j, P_k)_\psi^2 \quad \text{for } j \neq k; \quad (6)$$

neglecting the covariances $\Delta(X_j, P_k)_\psi$ for all j, k leads to the “naive” textbook inequalities

$$(\Delta X_j)_\psi (\Delta P_j)_\psi \geq \frac{1}{2}\hbar.$$

We are now going to rewrite Schrödinger's formulation (5), (6) of the position-momentum uncertainty principle in an equivalent, but obviously

symplectically covariant, way. For this purpose we introduce the “covariance matrix”

$$\Sigma = \begin{pmatrix} \Delta(X, X)_\psi & \Delta(X, P)_\psi \\ \Delta(P, X)_\psi & \Delta(P, P)_\psi \end{pmatrix} \quad (7)$$

where $\Delta(X, X)_\psi = ((\Delta X_j \Delta X_k)_\psi)_{1 \leq j, k \leq n}$, and so on.

Theorem 2 *The inequalities (5), (6) are equivalent to the following statement: the Hermitian matrix*

$$\Sigma + \frac{i\hbar}{2}J \text{ is positive semi-definite.} \quad (8)$$

Proof. See Narcowich and O’Connell [16], Narcowich [17] and Simon *et al.* [20, 21]. ■

The positive semi-definiteness of $\Sigma + \frac{i\hbar}{2}J$ implies that Σ itself is positive; in fact one can show that Σ is even positive-definite (see Narcowich [16]); this allows us to define the “Wigner ellipsoid”

$$\mathcal{W}_\Sigma : \frac{1}{2}\Sigma^{-1}z \cdot z \leq 1. \quad (9)$$

We will say that \mathcal{W}_Σ is *quantum mechanically admissible* when condition (8) is satisfied. This is a first step toward a geometrization of the uncertainty principle. Next step is gladly taken in the forthcoming section.

3 Uncertainty and Symplectic Capacities

A fundamental observation is now that condition (8) can be very simply stated in terms of an notion familiar from symplectic topology, namely the “symplectic capacity” of the Wigner ellipsoid (9). Recall (see for instance Hofer and Zehnder [12]) that a symplectic capacity on $(\mathbb{R}^{2n}, \sigma)$ is the assignment to every subset Ω of \mathbb{R}^{2n} of a number $c(\Omega) \geq 0$, or $+\infty$, such that the following conditions hold:

1. $c(f(\Omega)) = c(\Omega)$ for every symplectomorphism f of $(\mathbb{R}^{2n}, \sigma)$
2. $c(\Omega) \leq c(\Omega')$ if $\Omega \subset \Omega'$
3. $c(\lambda\Omega) = \lambda^2 c(\Omega)$ for every $\lambda \in \mathbb{R}$
4. $c(Z_j(r)) = c(B(r)) = \pi r^2$.

In Condition 4, $Z_j(r)$ and $B(r)$ are, respectively, the cylinder $x_j^2 + p_j^2 \leq r^2$ and the ball $|z| \leq r$. When we only allow linear or affine symplectomorphisms in Condition 1, we will talk about *linear symplectic capacities*. The existence of symplectic capacities is by no means easy to prove; all known constructions are notoriously difficult (see Hofer and Zehnder [12], Polterovich [18] for explicit examples of symplectic capacities). This difficulty is after all not so surprising, since the existence of a single symplectic capacity is equivalent to Gromov's non-squeezing theorem [9], which is a deep theorem of symplectic topology, whose proof requires sophisticated techniques (the theory of pseudo-holomorphic curves). Gromov's theorem says that there is no symplectomorphism f of $(\mathbb{R}^{2n}, \sigma)$ such that $f(B(R)) \subset Z_j(r)$ if $r < R$ (that such an f exists if $r \geq R$ is easy to prove). Defining, for $\Omega \subset \mathbb{R}^{2n}$,

$$c_G(\Omega) = \sup_{f \in \text{Symp}(n)} \{ \pi R^2 : f(B(R)) \subset \Omega \} \quad (10)$$

($\text{Symp}(n)$ the set of all symplectomorphisms of $(\mathbb{R}^{2n}, \sigma)$) it turns out that c_G indeed is a symplectic capacity ($c_G(\Omega)$ is sometimes called “Gromov's width” or “symplectic area” of Ω ; it can be proven that $c_G(\Omega)$ is the usual area when $n = 1$).

While there exist infinitely many symplectic capacities on $(\mathbb{R}^{2n}, \sigma)$ it turns out that all symplectic capacities agree on phase-space ellipsoids, and moreover agree with the linear symplectic capacity obtained by restricting f in (10) to affine symplectic transformations:

$$c_{\text{lin}}(\Omega) = \sup_{S \in I\text{Sp}(n, \mathbb{R})} \{ \pi R^2 : S(B(R)) \subset \Omega \}$$

where $I\text{Sp}(n, \mathbb{R})$ is the inhomogeneous symplectic group. Let us precise this result, and relate it to Williamson's theorem [22] (also see Hofer and Zehnder [12] for an alternative proof). That theorem says that one can diagonalize a positive-definite form using a symplectic matrix:

Theorem 3 (Williamson) *Let M be a positive definite $2n \times 2n$ real matrix and $Q(z) = Mz \cdot z$ the associated real quadratic form on \mathbb{R}^{2n} . Then there exists a symplectic matrix $S \in \text{Sp}(n, \mathbb{R})$ such that*

$$Q(Sz) = \sum_{j=1}^n \lambda_j (x_j^2 + p_j^2) \quad (11)$$

the positive numbers λ_j being the moduli of the eigenvalues $\pm i\lambda_j$ of JM .

It is customary to order the λ_j decreasingly: $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ and to call the finite sequence

$$\text{Spec}_\sigma(M) = (\lambda_1, \dots, \lambda_n)$$

the *symplectic spectrum* of Q (or of M). One proves the following properties:

$$\text{Spec}_\sigma(M^{-1}) = (\lambda_n^{-1}, \dots, \lambda_1^{-1}) \quad (12)$$

and

$$M \leq M' \implies \text{Spec}_\sigma(M) \leq \text{Spec}_\sigma(M') \quad (13)$$

(see *e.g.* de Gosson [5], Appendix, for a proof). The diagonalizing symplectic matrix S is of course not unique in general; however (ibid.) if S' is a second diagonalizing matrix then there exists $U \in \text{Sp}(n, \mathbb{R}) \cap O(2n)$ such that $S' = SU$ (or US).

It easily follows from Williamson's theorem and the properties of the symplectic spectrum that the linear symplectic capacity of the ellipsoid $\mathcal{Q} : Q(z) \leq 1$ is $c_{\text{lin}}(\mathcal{Q}) = \pi/\lambda_1$ and hence, since all symplectic capacities of an ellipsoid are equal,

$$c(\mathcal{Q}) = \frac{\pi}{\lambda_1}. \quad (14)$$

With this terminology the strong uncertainty principle can be restated in the following very concise form:

Theorem 4 *The uncertainty principle (5)-(6), and hence condition (8), are equivalent to the inequality*

$$c(\mathcal{W}_\Sigma) \geq \frac{1}{2}h \quad (15)$$

where c is any symplectic capacity (linear, or not) on $(\mathbb{R}^{2n}, \sigma)$ and \mathcal{W}_Σ is the Wigner ellipsoid (9).

Proof. It is a consequence of Williamson's theorem; see de Gosson [5, 7].

■

The inequality (15) tells us, in particular, that there exists $S \in \text{Sp}(n, \mathbb{R})$ sending the ball $B(\sqrt{h})$ in \mathcal{W}_Σ . The area of the section of $S(B(\sqrt{h}))$ by any plane of conjugate variables (or, more generally, by any symplectic plane) is equal to $\pi h = \frac{1}{2}h$: this is due to the fact that the restriction of a symplectomorphism to a symplectic subspace is still a symplectomorphism. As a consequence, we obtain the following geometric formulation of the uncertainty principle:

The intersection of a Wigner ellipsoid such that (15) holds by any symplectic plane cannot be inferior to $\frac{1}{2}h$.

It is interesting to note that we have the following dynamical interpretation of the results above. The Wigner ellipsoid \mathcal{W}_Σ can be viewed as the energy shell $H^{-1}(E)$ for the Hamiltonian function $H = \frac{1}{2}\Sigma^{-1}z \cdot z$ corresponding to the value $E = 1$. Symplectic capacities being symplectic invariants, it is no restriction to assume that Σ is in Williamson diagonal form, so that

$$H(z) = \sum_{j=1}^n \frac{\omega_j}{2} (x_j^2 + p_j^2)$$

where $(\omega_1, \dots, \omega_n)$ is the symplectic spectrum of Σ^{-1} . With these notations we have $c(\mathcal{W}_\Sigma) = \pi\omega_1$ so that the condition $c(\mathcal{W}_\Sigma) \geq \frac{1}{2}h$ can be rewritten as

$$\oint_{\gamma_1} p dx \geq \frac{1}{2}h$$

where γ_1 is the shortest periodic orbit carried by $H^{-1}(E)$ (namely, that lying in the x_1, p_1 plane).

4 Hardy's theorem and uncertainty

In what follows M will always denote a positive-definite real $2n \times 2n$ matrix. Recall [14] that the Wigner transform of a function $\psi \in L^2(\mathbb{R}^n)$ is defined by

$$W\psi(z) = \left(\frac{1}{2\pi\hbar}\right)^n \int e^{-\frac{i}{\hbar}p \cdot y} \psi\left(x + \frac{1}{2}y\right) \overline{\psi\left(x - \frac{1}{2}y\right)} dy$$

and that we have

$$\int W\psi(z) dp = |\psi(x)|^2 \quad , \quad \int W\psi(z) dx = |\mathcal{F}\psi(p)|^2. \quad (16)$$

The following theorem is a geometric formulation of Hardy's uncertainty principle:

Theorem 5 *Let $\psi \in L^2(\mathbb{R}^n)$, $\psi \neq 0$, and assume that there exists $C > 0$ such that $W\psi(z) \leq Ce^{-\frac{1}{\hbar}Mz \cdot z}$. Then $c(\mathcal{W}_\Sigma) \geq \frac{1}{2}h$ where \mathcal{W}_Σ is the Wigner ellipsoid corresponding to the choice $\Sigma = \frac{\hbar}{2}M^{-1}$ (equivalently $c(\mathcal{B}_M) \geq \frac{1}{2}h$ where $\mathcal{B}_M : Mz \cdot z \leq \hbar$).*

Proof. In view of Williamson's theorem we can find $S \in Sp(n, \mathbb{R})$ be such that

$$MSz \cdot Sz = \sum_{j=1}^n \lambda_j (x_j^2 + p_j^2)$$

with $\text{Spec}_\sigma(M) = (\lambda_1, \dots, \lambda_n)$ hence the assumption $W\psi(z) \leq Ce^{-\frac{1}{\hbar}Mz \cdot z}$ can be rewritten as

$$W\psi(S^{-1}z) \leq C \exp \left(-\frac{1}{\hbar} \sum_{j=1}^n \lambda_j (x_j^2 + p_j^2) \right). \quad (17)$$

Since $W\psi(S^{-1}z) = W\hat{S}\psi(z)$ where \hat{S} is any of the two operators in the metaplectic group $\text{Mp}(n, \mathbb{R})$ with projection S . Since $\hat{S}\psi \in L^2(\mathbb{R}^n)$ and $c(\mathcal{W}_\Sigma)$ is a symplectic invariant it is no restriction to assume $S = I$, $\hat{S} = I$. Integrating the inequality

$$W\psi(z) \leq C \exp \left(-\frac{1}{\hbar} \sum_{j=1}^n \lambda_j (x_j^2 + p_j^2) \right)$$

in x and p , respectively we get, using formulae (16),

$$|\psi(x)| \leq C_1 \exp \left(-\frac{1}{2\hbar} \sum_{j=1}^n \lambda_j x_j^2 \right) \quad (18)$$

$$|\mathcal{F}\psi(p)| \leq C_1 \exp \left(-\frac{1}{2\hbar} \sum_{j=1}^n \lambda_j p_j^2 \right) \quad (19)$$

for some constant $C_1 > 0$. Let us now introduce the following notation. We set $\psi_1(x_1) = \psi(x_1, 0, \dots, 0)$ and denote by \mathcal{F}_1 the one-dimensional Fourier transform in the x_1 variable. Now, we first note that (18) implies that

$$|\psi_1(x_1)| \leq C_1 \exp \left(-\frac{\lambda_1}{2\hbar} x_1^2 \right). \quad (20)$$

On the other hand, by definition of the Fourier transform \mathcal{F} ,

$$\int \mathcal{F}\psi(p) dp_2 \cdots dp_n = \left(\frac{1}{2\pi\hbar} \right)^{n/2} \int \int e^{-\frac{i}{\hbar}p \cdot x} \psi(x) dx dp_2 \cdots dp_n;$$

taking into account the Fourier inversion formula this is

$$\int \mathcal{F}\psi(p) dp_2 \cdots dp_n = (2\pi\hbar)^{(n-1)/2} \mathcal{F}_1 \psi_1(p_1).$$

It follows that

$$|\mathcal{F}_1\psi_1(p_1)| \leq \left(\frac{1}{2\pi\hbar}\right)^{(n-1)/2} C_1 \int e^{-\frac{1}{2\hbar} \sum_{j=1}^n \lambda_j p_j^2} dp_2 \cdots dp_n$$

that is

$$|\mathcal{F}_1\psi_1(p_1)| \leq C_3 \exp\left(-\frac{\lambda_1}{2\hbar} p_1^2\right) \quad (21)$$

for some constant $C_3 > 0$. Applying Hardy's theorem we see that the condition $\lambda_1^2 \leq 1$ is both necessary and sufficient for these inequalities to hold (remember that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$); in view of (14) this is the same thing as $c(\mathcal{B}_M) \geq \frac{1}{2}\hbar$. ■

5 The Case of "Quantum Blobs"

Let us look at the particular case where the ellipsoid $\mathcal{B}_M : Mz \cdot z$ is a "quantum blob", *i.e.* the image of the ball $B(\sqrt{\hbar})$ by a linear symplectic transformation (in which case we have $c(\mathcal{B}_M) = \frac{1}{2}\hbar$). We begin by shortly recalling some basic facts about the metaplectic group (for details and references see for instance Leray [13], or de Gosson [6, 8]).

The symplectic group $\mathrm{Sp}(n, \mathbb{R})$ is a connected classical Lie group, contractible to its maximal compact subgroup $U(n) = \mathrm{Sp}(n) \cap O(2n, \mathbb{R})$. The latter being diffeomorphic to $U(n, \mathbb{C})$ we have

$$\pi_1[\mathrm{Sp}(n)] \simeq \pi_1[U(n, \mathbb{C})] \simeq (\mathbb{Z}, +)$$

hence $\mathrm{Sp}(n, \mathbb{R})$ has covering groups $\mathrm{Sp}_q(n, \mathbb{R})$ of all orders $q = 2, 3, \dots, \infty$ and $\mathrm{Sp}_\infty(n, \mathbb{R})$ is its universal (= simply connected) covering. A particular role is played by the two-fold covering $\mathrm{Sp}_2(n, \mathbb{R})$, because it has a faithful representation as a subgroup of the unitary group of $L^2(\mathbb{R}^n)$, the *metaplectic group* $\mathrm{Mp}(n, \mathbb{R})$. The covering projection $\pi : \mathrm{Sp}_2(n) \longrightarrow \mathrm{Sp}(n)$ induces a two-to-one epimorphism $\pi_{\mathrm{Mp}} : \mathrm{Mp}(n, \mathbb{R}) \longrightarrow \mathrm{Sp}(n, \mathbb{R})$. The two elements of $\mathrm{Mp}(n, \mathbb{R})$ that cover $S \in \mathrm{Sp}(n, \mathbb{R})$ are denoted by \widehat{S} and $-\widehat{S}$.

In our context what we will need is the following "metaplectic covariance formula": let $W(\psi, \phi)$ be the Wigner–Moyal transform of the pair $(\psi, \phi) \in (L^2(\mathbb{R}^n))^2$. Then, for every $S \in \mathrm{Sp}(n, \mathbb{R})$ we have

$$W(\psi, \phi)(S^{-1}z) = W(\widehat{S}\psi, \widehat{S}\phi)(z) \quad (22)$$

where $\widehat{S} \in \mathrm{Mp}(n, \mathbb{R})$ is such that $\pi_{\mathrm{Mp}}(\widehat{S}) = S$.

With these notations, Theorem 5 has the following consequence:

Corollary 6 Assume that $\mathcal{B}_M = S(B(\sqrt{\hbar}))$ for some $S \in \text{Sp}(n, \mathbb{R})$. If $W\psi(z) \leq Ce^{-\frac{1}{\hbar}Mz \cdot z}$ then ψ is proportional to the squeezed coherent state $\hat{S}^{-1}\psi_0$ where $\psi_0(x) = (\pi\hbar)^{-n/4}e^{-\frac{1}{2\hbar}|x|^2}$ and \hat{S} is any of the two metaplectic operators $\pm\hat{S}$ covering S .

Proof. If $\mathcal{B}_M = S(B(\sqrt{\hbar}))$ then $\lambda_j = 1$ for all $j = 1, \dots, n$ and the inequality (17) in the proof of Theorem 5 can be written $W\psi(S^{-1}z) \leq Ce^{-\frac{1}{\hbar}|z|^2}$. Since $W\psi(S^{-1}z) = W\hat{S}\psi(z)$ in view of (22), Hardy's theorem now implies that $\hat{S}\psi(x) = (\pi\hbar)^{-n/4}e^{-\frac{1}{2\hbar}|x|^2}$ hence our claim. ■

6 Mixed states

Insofar we have been dealing with pure states; everything actually carries over without difficulty to the more general case of mixed states. Recall that a trace-class operator $\hat{\rho}$ on $L^2(\mathbb{R}^n)$ is called a *density operator* if it is positive (and hence self-adjoint) and has trace equal to one. It is advantageous to view $\hat{\rho}$ as a Weyl operator, in which case we can write

$$\hat{\rho}\psi(x) = \int \int e^{\frac{i}{\hbar}\langle p, x-y \rangle} \rho(\frac{1}{2}(x+y), p) \psi(y) dy dp;$$

the function ρ (which is $(2\pi\hbar)^n$ times the symbol of $\hat{\rho}$) is called the Wigner distribution of $\hat{\rho}$. The average value of a self-adjoint bounded operator A on $L^2(\mathbb{R}^n)$ with respect to $\hat{\rho}$ is then

$$\langle A \rangle_{\hat{\rho}} = \text{Tr}(\hat{\rho}A) = \int \rho(z)a(z)dz$$

(see Littlejohn [14] for a review of the notion). With these notations Schrödinger's form (4) of the uncertainty principle becomes

$$(\Delta A)_{\hat{\rho}}^2 (\Delta B)_{\hat{\rho}}^2 \geq \Delta(A, B)_{\hat{\rho}}^2 - \frac{1}{4} \langle [A, B] \rangle_{\hat{\rho}}^2 \quad (23)$$

where $(\Delta A)_{\hat{\rho}}^2$, etc. are defined exactly as in the “pure” case. These definitions extend to the case where the operators A and B are essentially self-adjoint; in practice they are required to be defined (at least) on the Schwartz space $\mathcal{S}(\mathbb{R}^n)$ of rapidly decreasing functions.

We will assume throughout that the function $z \mapsto (1 + |z|^2)\rho(z)$ is in $L^1(\mathbb{R}^{2n})$; then, in particular, we have the analogues of the uncertainty inequalities (5), (6):

$$(\Delta X_j)_{\hat{\rho}}^2 (\Delta P_j)_{\hat{\rho}}^2 \geq \Delta(X_j, P_j)_{\hat{\rho}}^2 + \frac{1}{4}\hbar^2, \quad 1 \leq j \leq n \quad (24)$$

$$(\Delta X_j)_{\hat{\rho}}^2 (\Delta P_k)_{\hat{\rho}}^2 \geq \Delta(X_j, P_k)_{\hat{\rho}}^2 \quad \text{for } j \neq k. \quad (25)$$

Writing $\Delta(X, X)_{\hat{\rho}} = ((\Delta X_j \Delta X_k)_{\hat{\rho}})_{1 \leq j, k \leq n}$, and so on, we call again the symmetric $2n \times 2n$ matrix

$$\Sigma = \begin{pmatrix} \Delta(X, X)_{\hat{\rho}} & \Delta(X, P)_{\hat{\rho}} \\ \Delta(P, X)_{\hat{\rho}} & \Delta(P, P)_{\hat{\rho}} \end{pmatrix} \quad (26)$$

the *covariance matrix* of the density operator $\hat{\rho}$.

The rub comes from the fact that the positivity of ρ does not guarantee that $\hat{\rho}$ is a non-negative operator (this is a peculiarity of the Weyl calculus to which much work and effort has been devoted: see for instance [2, 4] and the references therein). This apparent difficulty is actually a manifestation of the uncertainty principle; one proves (Narcowich [17] and Simon *et al.* [21]) that a necessary (but not sufficient!) condition for $\hat{\rho}$ to be a density operator is

$$M^{-1} + iJ \text{ is positive semi-definite.} \quad (27)$$

A simple calculation shows that we actually have $M = \frac{\hbar}{2}\Sigma^{-1}$ where Σ is the covariance matrix (26) so that condition (27) is just the strong form (8) of the uncertainty principle in Theorem 2.

The following result generalizes Theorem 5 to mixed states:

Theorem 7 *Let $M > 0$ and ρ be a smooth real function on \mathbb{R}^{2n} such that $\int \rho(z) dz = 1$. Assume that $\rho(z) \leq C e^{-\frac{1}{\hbar} M z \cdot z}$ for some $C \geq 0$ and consider the ellipsoid $\mathcal{B}_M : Mz \cdot z \leq \hbar$. If $c(\mathcal{B}_M) < \frac{1}{2}\hbar$ then ρ cannot be the Wigner distribution of any quantum state.*

Proof. As in the proof of Theorem 5 we can assume, taking into account Williamson's theorem and the invariance of symplectic capacities under canonical transformations, that

$$\rho(z) \leq \exp \left(-\frac{1}{\hbar} \sum_{j=1}^n \lambda_j (x_j^2 + p_j^2) \right). \quad (28)$$

Now there exists an orthonormal set of vectors $(\psi_j)_j$ in $L^2(\mathbb{R}^n)$ and numbers $\alpha_j \geq 0$, $\sum_j \alpha_j = 1$, such that

$$\rho(z) = \sum_j \alpha_j W\psi_j(z).$$

Integrating the inequality (28) in x and p , respectively we thus have

$$\begin{aligned}\sum_j \alpha_j \int W\psi_j(z)dp &\leq C_1 \exp\left(-\frac{1}{\hbar} \sum_{j=1}^n \lambda_j x_j^2\right) \\ \sum_j \alpha_j \int W\psi_j(z)dx &\leq C_1 \exp\left(-\frac{1}{\hbar} \sum_{j=1}^n \lambda_j p_j^2\right).\end{aligned}$$

Since $\int W\psi_j(z)dp = |\psi_j(x)|^2$ and $\int W\psi_j(z)dx = |\mathcal{F}\psi_j(p)|^2$ these inequalities imply in particular the existence of constants $C_j > 0$ such that

$$\begin{aligned}|\psi_j(x)| &\leq C_j \exp\left(-\frac{1}{2\hbar} \sum_{j=1}^n \lambda_j x_j^2\right) \\ |\mathcal{F}\psi_j(p)|^2 &\leq C_j \exp\left(-\frac{1}{2\hbar} \sum_{j=1}^n \lambda_j p_j^2\right).\end{aligned}$$

and one concludes as in the proof of Theorem 5. ■

As a consequence we get the following nonlocality result:

Corollary 8 *The Wigner distribution ρ of a quantum state cannot have compact support.*

Proof. Suppose that the support of ρ is contained in some ball $B(R) \subset \mathbb{R}^{2n}$. Let λ be a real number such that $0 < \lambda < 1$. We can find $C > 0$ such that $\rho(z) \leq Ce^{-\frac{1}{\hbar}\lambda|z|^2}$ for all z , which contradicts the statement in Theorem 7. ■

7 Conclusion and Conjectures

A question which we have not addressed in this Letter because of lack of space and timeliness is that of the relation between our constructions and deformation quantization [3]. deformation quantization is actually present everywhere in this work, if only as a watermark. For instance, our nonlocality statement of Corollary 8 (a Wigner distribution cannot have compact support) is related to the nonlocality of the star-product (intuitively the exponential of a Poisson bracket is a bidifferential operator of infinite order). This, and many other questions, certainly deserve a thorough investigation.

On a more pedestrian level, we remark that Gaussians $\psi(x) = Ce^{-\frac{1}{\hbar}Mz \cdot z}$ for which \mathcal{B}_M is a quantum blob correspond to the ground state of a generalized harmonic oscillator. A natural question is whether one could have similar results for the higher modes. The recent work [1] of Bonami, or its possible extensions, could play a crucial role in an answer to these questions.

Another natural extension would be the following: we have been dealing with non-degenerate Gaussians. It would be interesting to see what happens when W is of the type

$$W(z) = Ce^{-\frac{1}{\hbar}Mz \cdot z}$$

where M is positive semi-definite: $M \geq 0$. Williamson's diagonalization result (11) should then be replaced by the following statement: there exists $S \in \text{Sp}(n, \mathbb{R})$ and $k \leq n$, $\ell \leq n - k$ such that

$$Q(Sz) = \sum_{j=1}^k \lambda_j^\sigma (x_j^2 + p_j^2) + \sum_{j=k+1}^{k+\ell} x_j^2$$

where the $\pm i\lambda_j^\sigma$ ($\lambda_j^\sigma \geq 0$) are the eigenvalues of JM on the imaginary axis. In this case the inequality $Q(z) \leq \hbar$ no longer defines an ellipsoid, but rather a phase-space cylinder; it is easy to calculate the symplectic capacity of this cylinder, but how can this be related to the question whether W represents the Wigner distribution of some mixed quantum state?

Finally we wish to mention that Gröchenig and Zimmermann have obtained, in their discussion [11] of uncertainty principles for time-frequency representations, similar results by completely different methods for the short-time Fourier transform which is just the matrix coefficient of the Heisenberg group. Let $f, g \in L^2(\mathbb{R}^n)$. The *short-time Fourier transform* is defined as follows

$$V_g f(x, \xi) = \int_{\mathbb{R}^n} e^{-2\pi i \xi \cdot t} f(t) \overline{g(t - x)} dt \quad (29)$$

They showed that if $f \in S'(\mathbb{R}^n)$, $g \in S'(\mathbb{R}^n)$ satisfies

$$|V_g f(x, \xi)| = O(e^{-\pi(|x|^2 + |\xi|^2)})$$

as $|x|, |\xi| \rightarrow \infty$ then f and g are multiples of $e^{-2\pi i \xi_0 \cdot t} e^{-\pi(t - x_0)^2}$ for some (x_0, ξ_0) . The Wigner–Moyal distribution (3) of $(\psi, \phi) \in S'(\mathbb{R}^n) \times S'(\mathbb{R}^n)$ and the short-time Fourier transform (29) are related by the formula

$$W(\psi, \phi)(x, p) = \left(\frac{2}{\pi\hbar}\right)^{n/2} e^{\frac{2\pi i}{\hbar} p \cdot x} V_{g^\vee} f(x\sqrt{2/\pi\hbar}, p\sqrt{2/\pi\hbar})$$

where $f(x) = \psi(x\sqrt{2\pi\hbar})$, $g(x) = \phi(x\sqrt{2\pi\hbar})$, and $g^\vee(x) = g(-x)$, so that Gröchenig and Zimmermann's result can be restated as:

Assume that there exists $C > 0$ such that

$$|W(\psi, \phi)(z)| \leq Ce^{-\frac{1}{\hbar}|z|^2} \quad \text{for all } z = (x, p);$$

then we can find complex constants C_ψ and C_ϕ and $z_0 = (x_0, p_0)$ such that $\psi = C_\psi \widehat{T}(z_0)\psi_0$ and $\phi = C_\phi \widehat{T}(-z_0)\psi_0$ where ψ_0 is the standard coherent state $\psi_0(x) = (\pi\hbar)^{-n/4} e^{-\frac{1}{2\hbar}|x|^2}$.

Acknowledgement 9 *The authors would like to express their warmest thanks to Professor Daniel Sternheimer for valuable and interesting comments on earlier versions of this work, and for having drawn their attention to the relation between this work and deformation quantization.*

References

- [1] Bonami A., Demange B., and Jaming P.: Hermite functions and uncertainty principles for the Fourier and the windowed Fourier transform. *Rev. Mat. Iberoamericana* 19(1) 23–55 (2003)
- [2] Fefferman C. and Phong D. H.: The uncertainty principle and sharp Gårding inequalities. *Comm. Pure Appl. Math.* 75 285–331 (1981)
- [3] Bayen F., Flato M., Fronsdal C., Lichnerowicz A., and Sternheimer D.: Deformation Theory and Quantization. I. Deformation of Symplectic Structures. *Annals of Physics* 111, 6–110 (1978); II Physical Applications 110 111–151 (1978)
- [4] Folland G. B.: *Harmonic Analysis in Phase space*. *Annals of Mathematics studies*, Princeton University Press, Princeton, N. J. (1989)
- [5] de Gosson M.: Cellules quantiques symplectiques et fonctions de Husimi–Wigner. *Bull. Sci. Math.* 129 211–226 (2005)
- [6] de Gosson M.: On the Weyl Representation of Metaplectic Operators. *Letters in Mathematical Physics* 72 129–142 (2005)
- [7] de Gosson M.: Uncertainty Principle, Phase Space Ellipsoids and Weyl calculus. *Operator Theory: Advances and applications*. Vol. 164 121–132, Birkhäuser Verlag Basel (2006)
- [8] de Gosson M.: *Symplectic Geometry and Quantum Mechanics*. Birkhäuser, Basel, series “Operator Theory: Advances and Applications” (subseries: “Advances in Partial Differential Equations”) Vol. 166 (2006)

- [9] Gromov M.: Pseudoholomorphic curves in symplectic manifolds. Invent. Math. 82 307–347 (1985)
- [10] Hardy G. H.: A theorem concerning Fourier transforms. J. London. Math. Soc. 8 227–231 (1933)
- [11] Gröchenig K. and Zimmermann G.: Hardy’s theorem and the short-time Fourier transform of Schwartz functions. J. London. Math. Soc. (2) 63 205–214 (2001)
- [12] Hofer H. and Zehnder E.: Symplectic Invariants and Hamiltonian Dynamics. Birkhäuser Advanced texts (Basler Lehrbücher, Birkhäuser Verlag (1994)
- [13] Leray J.: Lagrangian Analysis and Quantum Mechanics, a mathematical structure related to asymptotic expansions and the Maslov index. Cambridge, MA: MIT Press (1981)
- [14] Littlejohn R. G.: The semiclassical evolution of wave packets. Physics Reports 138(4–5) 193–291 (1986)
- [15] Messiah A.: Mécanique Quantique. Dunod, Paris, 1961, Vol. 1 (1995) [English translation: Quantum Mechanics, North-Holland (1991)]
- [16] Narcowich F. J. and O’Connell R. F.: Necessary and sufficient conditions for a phase-space function to be a Wigner distribution. Phys. Rev. A 34(1) 1–6 (1986)
- [17] Narcowich F. J.: Geometry and uncertainty. J. Math. Phys. 31(2) (1990)
- [18] Polterovich L.: The Geometry of the Group of Symplectic Diffeomorphisms. Lectures in Mathematics, Birkhäuser (2001)
- [19] Radha R. and Thangavelu S.: Hardy’s inequalities for Hermite and Laguerre expansions. Proc. Am. Math. Soc. 132(12) 3525–3536 (2004)
- [20] Simon R., Sudarshan E. C. G., and Mukunda N.: Gaussian–Wigner distributions in quantum mechanics and optics. Phys. Rev. A 36(8) 3868–3880 (1987)
- [21] Simon R., Mukunda N., and Dutta B.: Quantum Noise Matrix for Multimode Systems: $U(n)$ -invariance, squeezing and normal forms. Phys. Rev. A 49 1567–1583 (1994)

- [22] Williamson J.: On the algebraic problem concerning the normal forms of linear dynamical systems. Amer. J. of Math. 58 141–163 (1936)